



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:42 AM UTC

PDB ID : 1FCF / pdb\_00001fcf  
Title : PHOTOSYSTEM II D1 C-TERMINAL PROCESSING PROTEASE  
Authors : Liao, D.I.; Qian, J.; Chisholm, D.A.; Jordan, D.B.; Diner, B.A.  
Deposited on : 2000-07-18  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

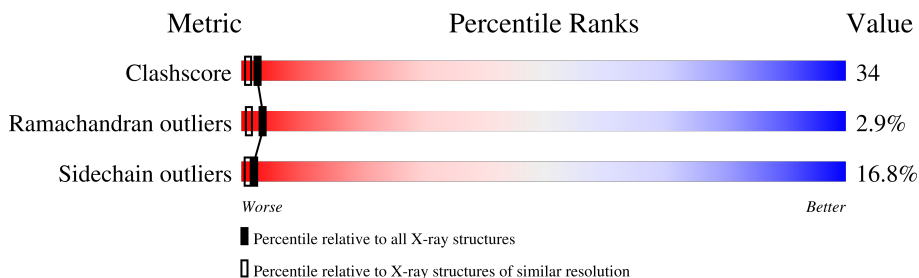
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	388	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3020 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PHOTOSYSTEM II D1 PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	387	2861	1791	506	559	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	initiating methionine	UNP O04073

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

- Molecule 3 is water.

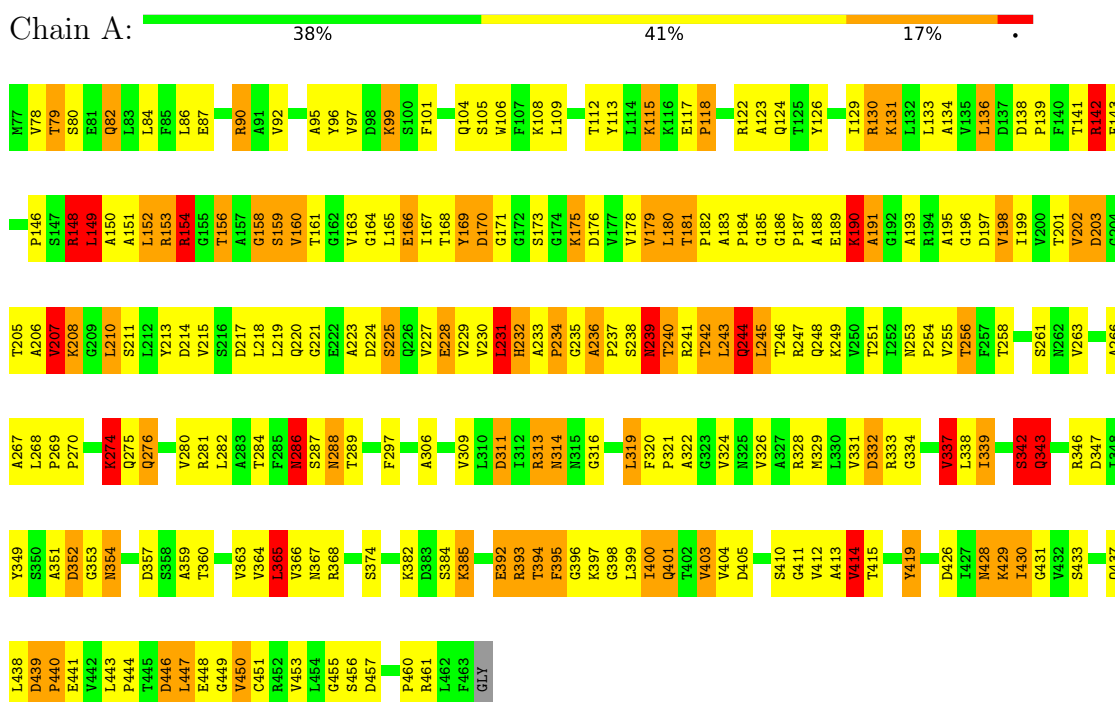
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	149	Total 149	O 149	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: PHOTOSYSTEM II D1 PROTEASE



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.75Å 148.75Å 100.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.10)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, $R_{free}$	0.220 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3020	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.55	12/2902 (0.4%)	2.07	95/3948 (2.4%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	441	GLU	CD-OE2	6.85	1.38	1.25
1	A	450	VAL	N-CA	-5.96	1.39	1.46
1	A	104	GLN	CA-C	-5.66	1.45	1.52
1	A	241	ARG	NE-CZ	5.36	1.39	1.33
1	A	447	LEU	N-CA	-5.34	1.40	1.46
1	A	446	ASP	C-N	-5.31	1.27	1.33
1	A	363	VAL	N-CA	-5.30	1.40	1.46
1	A	366	VAL	C-N	-5.23	1.28	1.33
1	A	284	THR	CA-C	-5.09	1.46	1.52
1	A	274	LYS	CA-C	-5.04	1.46	1.52
1	A	166	GLU	CD-OE2	5.03	1.34	1.25
1	A	363	VAL	CA-CB	-5.00	1.48	1.54

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	VAL	N-CA-C	11.27	124.54	109.21
1	A	153	ARG	N-CA-C	10.10	122.29	111.28
1	A	288	ASN	CA-CB-CG	-9.32	103.28	112.60
1	A	316	GLY	CA-C-N	-8.86	114.33	121.86
1	A	316	GLY	C-N-CA	-8.86	114.33	121.86
1	A	207	VAL	N-CA-C	8.56	121.12	112.90
1	A	203	ASP	CA-CB-CG	8.07	120.67	112.60
1	A	430	ILE	N-CA-C	7.65	118.44	110.72
1	A	365	LEU	N-CA-CB	7.38	122.34	110.16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	VAL	CB-CA-C	-7.21	102.64	111.08
1	A	170	ASP	N-CA-C	7.21	119.62	110.33
1	A	240	THR	N-CA-C	7.15	120.90	109.24
1	A	430	ILE	CA-C-N	-7.13	113.01	121.85
1	A	430	ILE	C-N-CA	-7.13	113.01	121.85
1	A	170	ASP	CA-CB-CG	-7.10	105.50	112.60
1	A	80	SER	CA-C-N	7.04	130.02	120.44
1	A	80	SER	C-N-CA	7.04	130.02	120.44
1	A	180	LEU	N-CA-C	-7.04	103.54	111.14
1	A	404	VAL	N-CA-CB	6.95	119.34	111.21
1	A	148	ARG	N-CA-CB	6.93	120.53	110.20
1	A	414	VAL	CB-CA-C	-6.86	99.94	110.50
1	A	170	ASP	CA-C-N	6.71	134.56	121.41
1	A	170	ASP	C-N-CA	6.71	134.56	121.41
1	A	244	GLN	CB-CA-C	6.64	121.18	110.29
1	A	457	ASP	CA-CB-CG	6.60	119.20	112.60
1	A	446	ASP	CA-CB-CG	-6.56	106.04	112.60
1	A	136	LEU	N-CA-CB	-6.56	100.11	110.28
1	A	243	LEU	CA-C-N	-6.44	112.38	121.72
1	A	243	LEU	C-N-CA	-6.44	112.38	121.72
1	A	401	GLN	CB-CA-C	-6.33	99.39	111.48
1	A	393	ARG	CG-CD-NE	6.22	125.68	112.00
1	A	154	ARG	N-CA-CB	6.09	120.79	110.49
1	A	82	GLN	CA-CB-CG	-6.00	102.09	114.10
1	A	395	PHE	N-CA-CB	5.92	118.77	109.94
1	A	414	VAL	N-CA-C	5.87	117.21	108.46
1	A	274	LYS	CB-CA-C	-5.87	98.75	110.42
1	A	314	ASN	CA-CB-CG	-5.84	106.76	112.60
1	A	176	ASP	N-CA-C	5.82	118.69	109.96
1	A	428	ASN	CA-CB-CG	-5.78	106.82	112.60
1	A	343	GLN	N-CA-C	5.77	119.93	113.01
1	A	118	PRO	N-CA-CB	5.71	108.10	103.36
1	A	342	SER	CA-C-N	5.68	132.43	121.18
1	A	342	SER	C-N-CA	5.68	132.43	121.18
1	A	220	GLN	CA-C-N	5.66	128.56	121.83
1	A	220	GLN	C-N-CA	5.66	128.56	121.83
1	A	280	VAL	CB-CA-C	-5.65	102.79	110.42
1	A	82	GLN	CB-CA-C	5.59	120.08	110.79
1	A	400	ILE	N-CA-CB	-5.55	104.46	111.46
1	A	149	LEU	CB-CA-C	5.55	121.28	110.57
1	A	451	CYS	CA-C-N	5.54	127.64	120.44
1	A	451	CYS	C-N-CA	5.54	127.64	120.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	VAL	N-CA-CB	5.52	116.74	110.72
1	A	313	ARG	N-CA-C	-5.52	103.24	110.53
1	A	366	VAL	CA-C-O	5.52	127.46	121.67
1	A	394	THR	CA-C-N	5.49	127.95	120.54
1	A	394	THR	C-N-CA	5.49	127.95	120.54
1	A	234	PRO	N-CA-CB	5.46	108.05	103.25
1	A	359	ALA	N-CA-C	5.45	120.58	113.88
1	A	392	GLU	CB-CG-CD	-5.43	103.36	112.60
1	A	364	VAL	N-CA-CB	-5.40	104.65	111.46
1	A	244	GLN	O-C-N	-5.40	116.38	123.02
1	A	191	ALA	CA-C-N	-5.40	114.11	122.69
1	A	191	ALA	C-N-CA	-5.40	114.11	122.69
1	A	239	ASN	OD1-CG-ND2	5.35	127.95	122.60
1	A	231	LEU	O-C-N	5.34	129.83	122.72
1	A	184	PRO	N-CA-CB	5.32	107.91	103.17
1	A	311	ASP	CA-C-O	5.29	126.12	120.46
1	A	337	VAL	CA-CB-CG2	5.28	119.38	110.40
1	A	115	LYS	N-CA-CB	5.28	117.63	109.98
1	A	263	VAL	CA-C-N	5.27	128.20	120.71
1	A	263	VAL	C-N-CA	5.27	128.20	120.71
1	A	403	VAL	CB-CA-C	-5.27	103.27	110.96
1	A	366	VAL	O-C-N	-5.27	117.19	123.04
1	A	396	GLY	N-CA-C	-5.26	106.45	115.08
1	A	352	ASP	N-CA-CB	5.25	118.23	110.56
1	A	220	GLN	N-CA-C	5.21	117.85	110.50
1	A	167	ILE	N-CA-C	5.21	116.81	108.89
1	A	430	ILE	N-CA-CB	-5.19	102.80	110.58
1	A	153	ARG	N-CA-CB	5.18	117.73	110.12
1	A	289	THR	N-CA-C	5.18	117.32	111.11
1	A	130	ARG	NE-CZ-NH2	-5.16	114.55	119.20
1	A	169	TYR	CA-C-O	-5.16	115.20	121.28
1	A	179	VAL	N-CA-CB	5.15	116.72	110.95
1	A	142	ARG	CA-CB-CG	5.14	124.37	114.10
1	A	297	PHE	CA-CB-CG	-5.08	108.72	113.80
1	A	228	GLU	O-C-N	5.07	129.12	123.19
1	A	173	SER	CB-CA-C	5.04	120.45	110.42
1	A	95	ALA	N-CA-C	5.03	119.55	113.41
1	A	244	GLN	CA-C-N	-5.03	114.78	122.62
1	A	244	GLN	C-N-CA	-5.03	114.78	122.62
1	A	419	TYR	CB-CA-C	-5.03	101.24	109.53
1	A	286	ASN	CA-CB-CG	5.02	117.62	112.60
1	A	225	SER	N-CA-CB	5.02	118.16	110.49

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	GLY	N-CA-C	-5.01	107.84	115.66
1	A	236	ALA	O-C-N	5.00	127.07	121.32

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2861	0	2902	195	1
2	A	10	0	0	0	0
3	A	149	0	0	16	1
All	All	3020	0	2902	195	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (195) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:VAL:HG22	1:A:242:THR:HG23	1.42	0.98
1:A:286:ASN:ND2	1:A:288:ASN:H	1.62	0.97
1:A:398:GLY:H	1:A:428:ASN:HD22	1.02	0.95
1:A:256:THR:HG23	1:A:447:LEU:HD21	1.51	0.93
1:A:243:LEU:HB3	1:A:245:LEU:HD21	1.50	0.92
1:A:175:LYS:HB3	1:A:208:LYS:HD3	1.57	0.87
1:A:286:ASN:HD21	1:A:288:ASN:HB2	1.40	0.86
1:A:161:THR:HG22	1:A:249:LYS:HG3	1.57	0.85
1:A:243:LEU:CB	1:A:245:LEU:HD21	2.05	0.85
1:A:309:VAL:CG1	1:A:365:LEU:HD21	2.08	0.83
1:A:186:GLY:O	1:A:190:LYS:HG3	1.80	0.81
1:A:438:LEU:O	1:A:440:PRO:HD3	1.80	0.81
1:A:286:ASN:HD22	1:A:288:ASN:H	1.28	0.81
1:A:398:GLY:H	1:A:428:ASN:ND2	1.80	0.79
1:A:365:LEU:HD23	1:A:365:LEU:N	1.98	0.78

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLY:N	1:A:428:ASN:HD22	1.79	0.77
1:A:412:VAL:HG12	1:A:414:VAL:HG22	1.69	0.74
1:A:153:ARG:HH22	1:A:403:VAL:HB	1.53	0.73
1:A:211:SER:O	1:A:215:VAL:HG23	1.88	0.73
1:A:235:GLY:C	1:A:237:PRO:HD3	2.13	0.73
1:A:309:VAL:HG12	1:A:365:LEU:HD21	1.71	0.72
1:A:165:LEU:CD2	1:A:179:VAL:HG22	2.20	0.72
1:A:99:LYS:N	1:A:342:SER:OG	2.20	0.72
1:A:244:GLN:C	1:A:245:LEU:HD23	2.15	0.72
1:A:208:LYS:HB2	3:A:573:HOH:O	1.90	0.72
1:A:189:GLU:C	1:A:191:ALA:H	1.99	0.70
1:A:153:ARG:NH2	1:A:403:VAL:HB	2.05	0.70
1:A:202:VAL:HG11	1:A:219:LEU:HD23	1.73	0.70
1:A:196:GLY:O	1:A:234:PRO:HG3	1.93	0.69
1:A:367:ASN:HA	1:A:392:GLU:HG2	1.75	0.69
1:A:202:VAL:HG13	1:A:229:VAL:HG22	1.74	0.68
1:A:238:SER:O	1:A:240:THR:N	2.26	0.68
1:A:165:LEU:HD21	1:A:179:VAL:HG22	1.75	0.68
1:A:443:LEU:HD23	1:A:453:VAL:HG11	1.74	0.67
1:A:170:ASP:CG	1:A:171:GLY:H	2.03	0.67
1:A:382:LYS:NZ	1:A:433:SER:O	2.27	0.67
1:A:163:VAL:HG21	1:A:245:LEU:HD12	1.78	0.66
1:A:148:ARG:O	1:A:152:LEU:HB3	1.94	0.66
1:A:334:GLY:N	3:A:505:HOH:O	2.26	0.66
1:A:430:ILE:HG22	1:A:431:GLY:O	1.96	0.66
1:A:243:LEU:HB3	1:A:245:LEU:CD2	2.24	0.65
1:A:154:ARG:HD2	1:A:154:ARG:N	2.09	0.65
1:A:286:ASN:HD22	1:A:286:ASN:C	2.05	0.65
1:A:133:LEU:O	1:A:136:LEU:HB2	1.96	0.65
1:A:365:LEU:HD23	1:A:365:LEU:H	1.60	0.65
1:A:158:GLY:C	1:A:160:VAL:H	2.06	0.64
1:A:229:VAL:O	1:A:243:LEU:N	2.28	0.64
1:A:256:THR:CG2	1:A:447:LEU:HD21	2.28	0.63
1:A:337:VAL:HG23	1:A:349:TYR:HB2	1.81	0.63
1:A:148:ARG:HH11	1:A:148:ARG:HG3	1.63	0.63
1:A:229:VAL:HG12	1:A:231:LEU:HD23	1.81	0.62
1:A:207:VAL:HA	1:A:210:LEU:HD12	1.81	0.62
1:A:179:VAL:HG11	1:A:182:PRO:HD3	1.82	0.61
1:A:148:ARG:NH2	1:A:217:ASP:OD2	2.34	0.61
1:A:149:LEU:HD12	1:A:153:ARG:HE	1.65	0.60
1:A:354:ASN:H	1:A:354:ASN:HD22	1.49	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:LEU:HD11	1:A:443:LEU:HD12	1.83	0.59
1:A:141:THR:HA	1:A:413:ALA:O	2.03	0.59
1:A:266:ALA:O	1:A:461:ARG:HA	2.03	0.59
1:A:149:LEU:CD1	1:A:153:ARG:HE	2.15	0.59
1:A:134:ALA:HB3	3:A:561:HOH:O	2.03	0.58
1:A:343:GLN:O	1:A:343:GLN:HG2	2.03	0.58
1:A:286:ASN:ND2	1:A:288:ASN:N	2.42	0.58
1:A:189:GLU:O	1:A:191:ALA:N	2.37	0.58
1:A:426:ASP:OD1	1:A:429:LYS:HG3	2.04	0.57
1:A:351:ALA:HB3	3:A:505:HOH:O	2.05	0.57
1:A:448:GLU:HG2	3:A:603:HOH:O	2.03	0.57
1:A:139:PRO:HB2	1:A:169:TYR:CE1	2.39	0.57
1:A:286:ASN:HD22	1:A:288:ASN:N	1.98	0.56
1:A:178:VAL:HG12	1:A:198:VAL:HG22	1.87	0.56
1:A:232:HIS:HD2	1:A:233:ALA:O	1.89	0.56
1:A:236:ALA:HB1	1:A:239:ASN:HB2	1.87	0.56
1:A:351:ALA:N	3:A:505:HOH:O	2.36	0.56
1:A:210:LEU:HD22	1:A:214:ASP:HB3	1.88	0.56
1:A:384:SER:O	1:A:385:LYS:HB2	2.04	0.56
1:A:397:LYS:O	1:A:397:LYS:HG2	2.06	0.56
1:A:229:VAL:CG1	1:A:231:LEU:HD23	2.36	0.55
1:A:158:GLY:O	1:A:160:VAL:N	2.39	0.54
1:A:339:ILE:HG13	1:A:347:ASP:HB3	1.88	0.54
1:A:232:HIS:CD2	1:A:233:ALA:O	2.61	0.54
1:A:352:ASP:OD1	1:A:354:ASN:ND2	2.41	0.54
1:A:223:ALA:O	1:A:224:ASP:HB2	2.07	0.54
1:A:130:ARG:HG2	3:A:508:HOH:O	2.06	0.54
1:A:229:VAL:HG12	1:A:231:LEU:CD2	2.37	0.54
1:A:115:LYS:HD3	1:A:115:LYS:N	2.22	0.53
1:A:309:VAL:HG13	1:A:365:LEU:HD21	1.88	0.53
1:A:243:LEU:HB2	1:A:245:LEU:HD21	1.87	0.53
1:A:256:THR:HG21	3:A:528:HOH:O	2.08	0.53
1:A:97:VAL:HG11	1:A:415:THR:HG22	1.91	0.53
1:A:319:LEU:HD23	1:A:321:PRO:HG2	1.90	0.53
1:A:326:VAL:O	1:A:329:MET:HB2	2.09	0.52
1:A:148:ARG:C	1:A:150:ALA:H	2.18	0.52
1:A:203:ASP:OD2	1:A:227:VAL:HG23	2.09	0.51
1:A:97:VAL:HG11	1:A:415:THR:CG2	2.40	0.51
1:A:324:VAL:O	1:A:328:ARG:HG3	2.10	0.51
1:A:179:VAL:CG1	1:A:182:PRO:HD3	2.40	0.51
1:A:218:LEU:HD23	3:A:607:HOH:O	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:LEU:HB2	3:A:596:HOH:O	2.09	0.51
1:A:149:LEU:HD22	1:A:411:GLY:HA3	1.92	0.51
1:A:163:VAL:O	1:A:188:ALA:HB2	2.11	0.50
1:A:149:LEU:HG	1:A:149:LEU:O	2.11	0.50
1:A:189:GLU:C	1:A:191:ALA:N	2.65	0.50
1:A:229:VAL:CG1	1:A:231:LEU:CD2	2.89	0.50
1:A:139:PRO:HB2	1:A:169:TYR:CD1	2.47	0.50
1:A:255:VAL:HA	1:A:281:ARG:O	2.11	0.50
1:A:320:PHE:N	1:A:321:PRO:HD2	2.27	0.49
1:A:130:ARG:HH11	1:A:143:PHE:HD2	1.61	0.49
1:A:253:ASN:OD1	1:A:254:PRO:HD2	2.13	0.49
1:A:246:THR:O	1:A:248:GLN:HG3	2.12	0.48
1:A:365:LEU:N	1:A:365:LEU:CD2	2.74	0.48
1:A:149:LEU:HD13	1:A:403:VAL:HG11	1.94	0.48
1:A:163:VAL:O	1:A:163:VAL:HG23	2.14	0.48
1:A:113:TYR:HE2	1:A:131:LYS:HB3	1.78	0.48
1:A:365:LEU:CD1	1:A:443:LEU:HD12	2.43	0.48
1:A:96:TYR:O	1:A:99:LYS:HE3	2.14	0.48
1:A:138:ASP:OD2	1:A:415:THR:OG1	2.23	0.47
1:A:146:PRO:HD3	1:A:410:SER:HB3	1.95	0.47
1:A:196:GLY:C	1:A:234:PRO:HG3	2.39	0.47
1:A:286:ASN:C	1:A:319:LEU:HD13	2.39	0.47
1:A:84:LEU:HD22	1:A:122:ARG:HD2	1.97	0.47
1:A:84:LEU:O	1:A:87:GLU:HB2	2.15	0.47
1:A:101:PHE:CD1	1:A:106:TRP:HB2	2.50	0.47
1:A:170:ASP:CG	1:A:171:GLY:N	2.71	0.47
1:A:367:ASN:O	1:A:394:THR:HA	2.13	0.47
1:A:385:LYS:HE3	3:A:514:HOH:O	2.15	0.47
1:A:395:PHE:HD2	1:A:397:LYS:HB2	1.80	0.47
1:A:207:VAL:O	1:A:210:LEU:HB2	2.15	0.47
1:A:446:ASP:O	1:A:450:VAL:HG23	2.14	0.47
1:A:113:TYR:CE2	1:A:131:LYS:HD3	2.50	0.46
1:A:267:ALA:HB2	1:A:460:PRO:O	2.15	0.46
1:A:105:SER:HB3	1:A:108:LYS:HB3	1.98	0.46
1:A:444:PRO:O	1:A:450:VAL:HG22	2.14	0.46
1:A:197:ASP:HA	1:A:234:PRO:HD3	1.97	0.46
1:A:368:ARG:HB3	3:A:564:HOH:O	2.16	0.46
1:A:213:TYR:O	1:A:217:ASP:OD2	2.34	0.46
1:A:225:SER:OG	1:A:247:ARG:HD2	2.16	0.46
1:A:136:LEU:HD23	1:A:136:LEU:HA	1.56	0.45
1:A:401:GLN:HA	1:A:415:THR:HA	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ALA:HB1	1:A:239:ASN:CB	2.46	0.45
1:A:258:THR:HG22	1:A:447:LEU:HD22	1.99	0.45
1:A:97:VAL:CG1	1:A:415:THR:HG22	2.47	0.45
1:A:118:PRO:O	1:A:124:GLN:HB3	2.16	0.45
1:A:405:ASP:HB3	3:A:566:HOH:O	2.17	0.45
1:A:446:ASP:OD2	1:A:449:GLY:N	2.44	0.45
1:A:195:ALA:HB2	1:A:314:ASN:HD21	1.82	0.44
1:A:139:PRO:HD2	3:A:540:HOH:O	2.17	0.44
1:A:242:THR:O	1:A:243:LEU:HD23	2.17	0.44
1:A:159:SER:HA	1:A:249:LYS:NZ	2.33	0.44
1:A:268:LEU:HA	1:A:268:LEU:HD23	1.74	0.44
1:A:92:VAL:HG13	1:A:96:TYR:HB2	2.00	0.44
1:A:244:GLN:O	1:A:245:LEU:HD23	2.18	0.43
1:A:202:VAL:HG13	1:A:229:VAL:CG2	2.46	0.43
1:A:332:ASP:O	1:A:353:GLY:HA2	2.18	0.43
1:A:195:ALA:HB2	1:A:314:ASN:ND2	2.33	0.43
1:A:205:THR:HG22	1:A:206:ALA:O	2.19	0.43
1:A:245:LEU:HD23	1:A:245:LEU:N	2.32	0.43
1:A:187:PRO:HB3	3:A:576:HOH:O	2.19	0.42
1:A:198:VAL:CG1	1:A:199:ILE:N	2.80	0.42
1:A:164:GLY:HA3	1:A:183:ALA:HB3	2.01	0.42
1:A:185:GLY:N	1:A:189:GLU:OE1	2.27	0.42
1:A:412:VAL:CG1	1:A:414:VAL:HG22	2.43	0.42
1:A:333:ARG:NH2	3:A:594:HOH:O	2.49	0.42
1:A:79:THR:OG1	1:A:82:GLN:HG3	2.20	0.42
1:A:153:ARG:NH2	1:A:403:VAL:CB	2.78	0.42
1:A:148:ARG:C	1:A:150:ALA:N	2.78	0.42
1:A:221:GLY:CA	1:A:247:ARG:CD	2.97	0.42
1:A:400:ILE:HD11	1:A:419:TYR:CE2	2.54	0.42
1:A:106:TRP:CE3	1:A:106:TRP:HA	2.55	0.41
1:A:123:ALA:O	1:A:126:TYR:HB2	2.20	0.41
1:A:221:GLY:HA3	1:A:247:ARG:CD	2.49	0.41
1:A:331:VAL:O	1:A:351:ALA:HB1	2.21	0.41
1:A:232:HIS:CD2	1:A:232:HIS:C	2.96	0.41
1:A:392:GLU:HB3	1:A:440:PRO:HG3	2.02	0.41
1:A:166:GLU:OE2	1:A:181:THR:HG22	2.20	0.41
1:A:313:ARG:NH1	1:A:443:LEU:O	2.46	0.41
1:A:168:THR:HG23	1:A:169:TYR:N	2.34	0.41
1:A:86:LEU:O	1:A:90:ARG:HB2	2.20	0.41
1:A:105:SER:O	1:A:109:LEU:HD13	2.20	0.41
1:A:190:LYS:HB2	1:A:190:LYS:HE2	1.59	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LYS:HB2	1:A:430:ILE:H	1.37	0.41
1:A:354:ASN:HD22	1:A:354:ASN:N	2.11	0.41
1:A:142:ARG:N	1:A:413:ALA:O	2.47	0.40
1:A:311:ASP:OD1	1:A:313:ARG:HG3	2.21	0.40
1:A:357:ASP:OD2	1:A:360:THR:OG1	2.28	0.40
1:A:148:ARG:HA	1:A:151:ALA:HB3	2.03	0.40
1:A:276:GLN:O	1:A:306:ALA:HB3	2.21	0.40
1:A:117:GLU:HA	1:A:118:PRO:HD3	1.92	0.40
1:A:129:ILE:O	1:A:133:LEU:HG	2.22	0.40
1:A:188:ALA:O	1:A:193:ALA:HB3	2.22	0.40
1:A:221:GLY:N	1:A:247:ARG:NE	2.70	0.40
1:A:395:PHE:CD2	1:A:397:LYS:HB2	2.56	0.40
1:A:322:ALA:O	1:A:326:VAL:HG23	2.21	0.40
1:A:453:VAL:O	1:A:456:SER:OG	2.28	0.40
1:A:165:LEU:HD22	1:A:179:VAL:HG22	1.98	0.40
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.72	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:513:HOH:O	3:A:513:HOH:O[5_555]	1.84	0.36
1:A:439:ASP:OD1	1:A:439:ASP:OD1[10_545]	1.89	0.31

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	385/388 (99%)	350 (91%)	24 (6%)	11 (3%)	<b>3</b> <b>1</b>

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	THR
1	A	159	SER
1	A	190	LYS
1	A	239	ASN
1	A	274	LYS
1	A	440	PRO
1	A	439	ASP
1	A	99	LYS
1	A	270	PRO
1	A	158	GLY
1	A	269	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	303/303 (100%)	252 (83%)	51 (17%)	<b>2</b> <b>1</b>

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	THR
1	A	90	ARG
1	A	112	THR
1	A	131	LYS
1	A	142	ARG
1	A	148	ARG
1	A	149	LEU
1	A	152	LEU
1	A	154	ARG
1	A	156	THR
1	A	160	VAL
1	A	175	LYS
1	A	180	LEU
1	A	181	THR
1	A	190	LYS
1	A	201	THR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	202	VAL
1	A	207	VAL
1	A	208	LYS
1	A	210	LEU
1	A	228	GLU
1	A	231	LEU
1	A	232	HIS
1	A	242	THR
1	A	244	GLN
1	A	245	LEU
1	A	251	THR
1	A	256	THR
1	A	261	SER
1	A	274	LYS
1	A	275	GLN
1	A	276	GLN
1	A	282	LEU
1	A	286	ASN
1	A	287	SER
1	A	319	LEU
1	A	332	ASP
1	A	337	VAL
1	A	338	LEU
1	A	339	ILE
1	A	342	SER
1	A	343	GLN
1	A	346	ARG
1	A	354	ASN
1	A	365	LEU
1	A	374	SER
1	A	385	LYS
1	A	393	ARG
1	A	414	VAL
1	A	429	LYS
1	A	437	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	82	GLN
1	A	102	ASN
1	A	104	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	232	HIS
1	A	286	ASN
1	A	303	GLN
1	A	354	ASN
1	A	428	ASN
1	A	437	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	465	-	4,4,4	0.97	0	6,6,6	1.03	1 (16%)
2	SO4	A	466	-	4,4,4	1.28	0	6,6,6	0.96	1 (16%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	465	SO4	O4-S-O3	2.07	119.94	108.54
2	A	466	SO4	O4-S-O3	2.00	119.59	108.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.